

SAMRAI

*Structured Adaptive Mesh
Refinement Application
Infrastructure*

Technology

SAMRAI is an object-oriented software framework for structured adaptive mesh refinement (AMR) research. SAMRAI provides computational scientists with general and extensible support for rapid prototyping and development of parallel structured AMR applications. The primary goal of the SAMRAI effort is to facilitate numerical method and solution algorithm development for AMR applications that require high-performance computing hardware.

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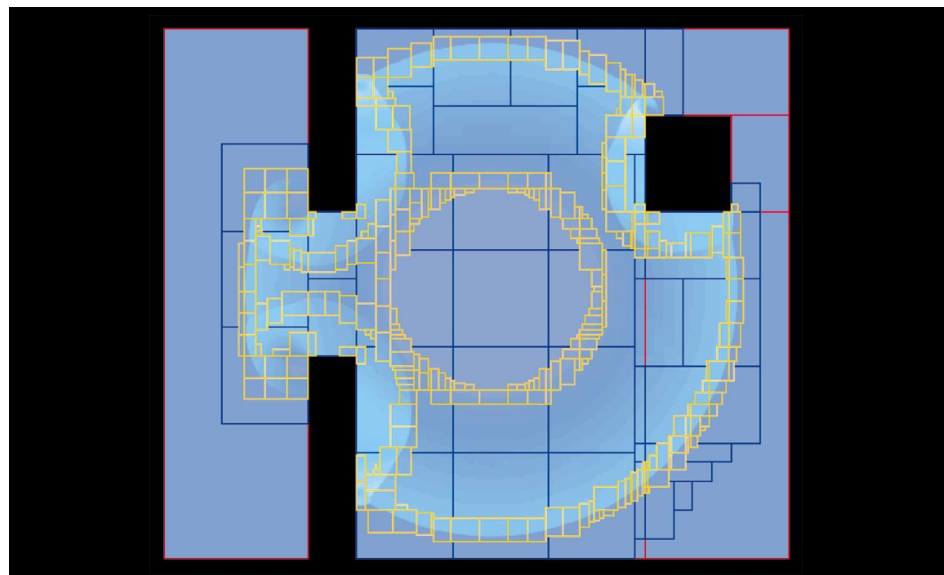


Figure 1. Adaptive mesh refinement concentrates computational effort in areas of interest, such as near the shock fronts in this hydrodynamics simulation.

Developments in high-performance computing hardware make it possible to simulate large three-dimensional problems that model increasingly complex chemical and physical processes. However, the numerical resolution required to capture the phenomena represented by mathematical models still makes such computations very expensive. In many interesting science and engineering applications, the most important features of the simulation occur in localized regions of the computational domain. Uniformly fine computational meshes that resolve the local phenomena may be unnecessarily fine outside the regions of interest. As a result, such uniform grid simulations can be inefficient or even prohibitively expensive.

Structured AMR provides a systematic way to focus computational resources (CPU time and memory) by employing varying degrees of local spatial and temporal resolution. Thus, AMR is an important technology needed to support large-scale, physically and numerically well-resolved, three-dimensional simulations.

Emerging AMR Application Domains

Structured AMR has proved to be a useful simulation technology for many fluid dynamics applications (Figure 1). SAMRAI is being developed as a substantial generalization of existing AMR technology. In addition to supporting more traditional AMR applications, SAMRAI is designed to explore new problem areas and new AMR solution algorithms. New applications include, but are not limited to, problems modeled by coupled systems of partial differential equations that exhibit complicated combinations of hyperbolic, elliptic, and parabolic behavior (such as radiation hydrodynamics, flow and transport in porous media, combustion, and reactive transport), neutron transport, hybrid models that combine discrete and continuum numerical models, and Arbitrary Lagrangian-Eulerian (ALE) integration methods.

The application of structured AMR to such problems gives rise to many interesting algorithmic, numerical, and computer science research questions. These issues are related to mathematical model approximations in an AMR

setting, adaptive integration methods, load balancing for distributed memory parallel computing, and software framework design and development. SAMRAI currently supports a variety of computational science projects. Through collaborations with researchers at DOE laboratories and universities, we are investigating the application of AMR technology to some of the application domains mentioned previously.

The SAMRAI Framework

Numerical algorithms for AMR problems are complex and require a substantial amount of software infrastructure. However, many software components used in AMR codes are similar across a broad spectrum of applications. These common components can be incorporated into a single general-purpose application framework. SAMRAI is being developed for two purposes: first, to codify existing AMR software support into a flexible, extensible, parallel development framework; and second, to apply structured AMR technology to new problem domains and to develop alternative

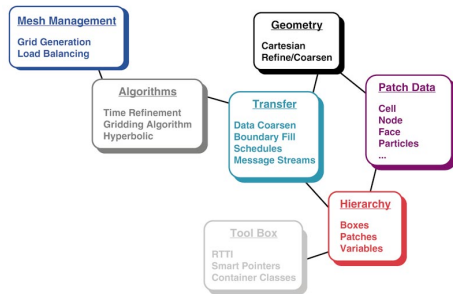


Figure 2. The SAMRAI framework consists of a collection of software components that greatly simplify the development of structured AMR applications.

adaptive solution algorithms for more traditional applications.

Since AMR applications involve complex, dynamically changing data communication patterns, it is particularly challenging on parallel computers. From its inception, SAMRAI was designed to facilitate sophisticated numerical algorithm development in a parallel computing environment. Three main software design points SAMRAI addresses are: first, support for a wide range of complex data structures on an adaptively-refined mesh, including arbitrary user-defined types; second, algorithmic flexibility, extensibility, and software reuse; and third, general software support for parallel application development.

SAMRAI facilitates rapid prototyping of various application code implementation alternatives by freeing developers from low-level data structure and algorithm management. An application developer views SAMRAI as a collection of software packages and classes that may be combined in complex ways to build an application (Figure 2). We use object-oriented design techniques so that many fundamental SAMRAI components may be enhanced without changing the underlying framework source code or re-compiling the library. In particular, software components may be specialized and extended through C++ class derivation. We are also addressing

interoperability issues that will allow applications built using SAMRAI to take advantage of other software packages, such as linear and nonlinear solver libraries, including PETSc, KINSOL, and *hypra*.

SAMRAI's framework structure provides flexibility to explore a wide range of AMR applications. Its design helps to reduce code development, encourages interoperability in application software, and simplifies the learning curve for new adaptive computational methods. Finally, SAMRAI provides robust support for parallelism to insulate communication operations from application code without impeding performance.

SAMRAI Applications and Framework Validation

In collaboration with researchers, we are using SAMRAI across a diverse range of applications. We are collaborating with academic researchers to employ SAMRAI in an application that couples fluid dynamics models (including turbulence and reactive chemistry) to container dynamics models to study firespread problems. Another SAMRAI applications code combines plasma fluid simulation with a model for laser light propagation. Other projects include simulation of solar winds in the Earth's magnetosphere, radiation-hydrodynamics using ALE integration methods, shear band formation in granular materials, flow and transport in porous media, neutron transport, and multi-physics problems that combine continuum and discrete particle models.

Each application emphasizes the combination of different numerical models and solution techniques in the context of structured AMR. For example, the firespread application uses both implicit and explicit integration methods for fluid calculations that are coupled to particle-like methods to model solid

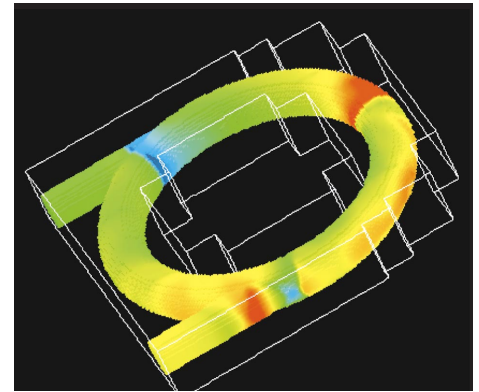


Figure 3. Embedded boundary capabilities enable structured AMR applications to capture complex geometry in an efficient manner.

containers. The solar wind problem combines magneto-hydrodynamics equations with a dipole field model of the Earth's ionosphere.

In addition to producing interesting computational science research, these applications serve as a validation of the SAMRAI software architecture, as they require substantial data structure and algorithmic flexibility. The applications produce a variety of simulation data on an adaptive mesh, including particles and embedded interfaces (Figure 3), as well as various forms of array-based data. Also, these complex solution algorithms combine sophisticated numerical methods to treat different aspects of each problem. Finally, incorporation of linear and nonlinear solution software tests SAMRAI's ability to interoperate with independently developed solver libraries.

For additional information about the SAMRAI project, visit the Web site at <http://www.llnl.gov/CASC/SAMRAI> or contact:

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